

An optimized buffer system for NMR-based urinary metabonomics with effective pH control, chemical shift consistency and dilution minimization

Chaoni Xiao^{1,2}, Fuhua Hao¹, Xiaorong Qin³, Yulan Wang^{1*}, Huiru Tang^{1*}

¹State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics, Wuhan Centre for Magnetic Resonance, Wuhan Institute of Physics and Mathematics, the Chinese Academy of Sciences, Wuhan 430071, P. R. China

²Graduate School of the Chinese Academy of Sciences, Beijing 100049, P.R. China

³ College of Chemical Engineering and Technology, Wuhan University of Science and Technology, Wuhan 430081, P.R. China

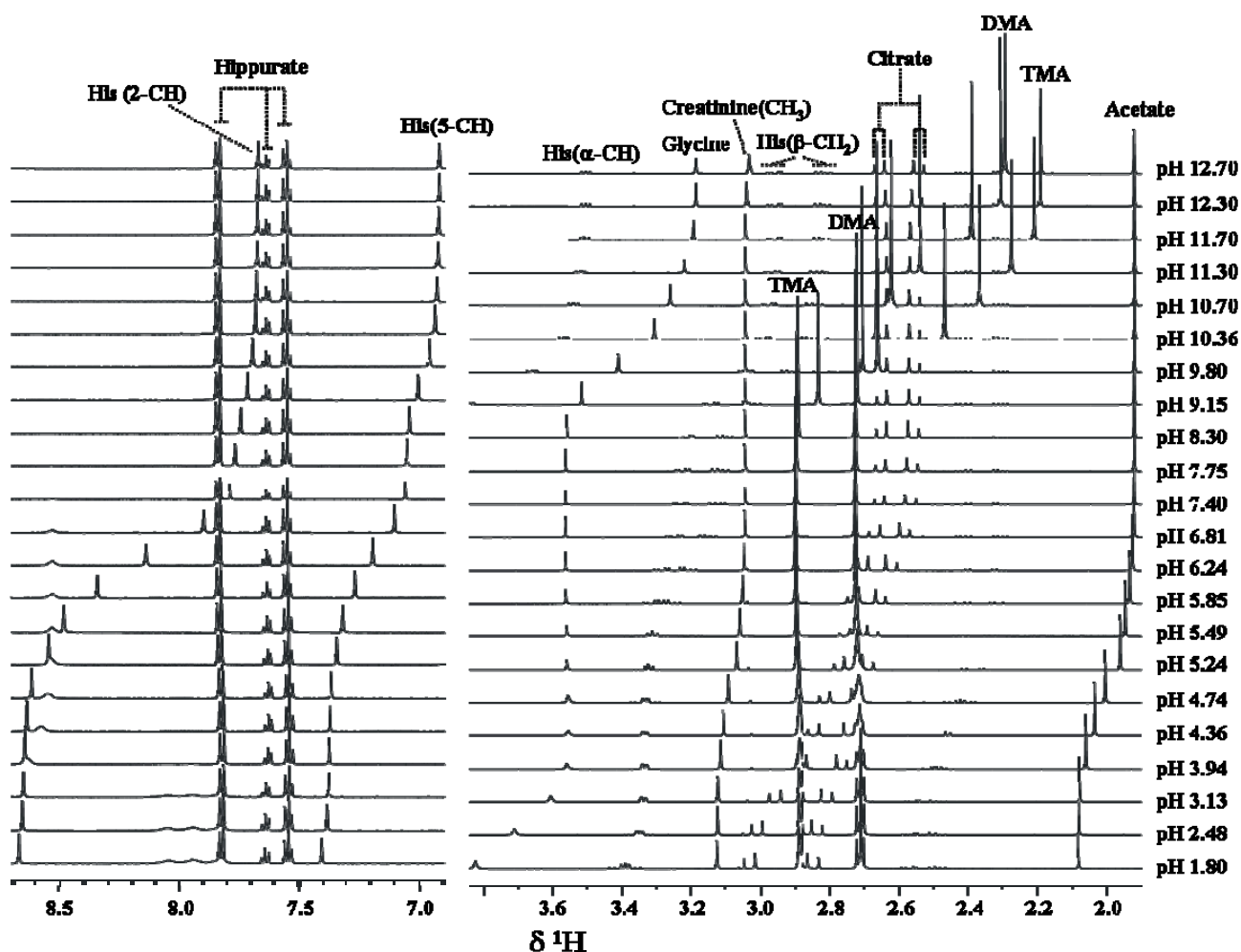


Figure S-1. The ¹H NMR spectra for the mixture solutions with different pH values at zero salt.

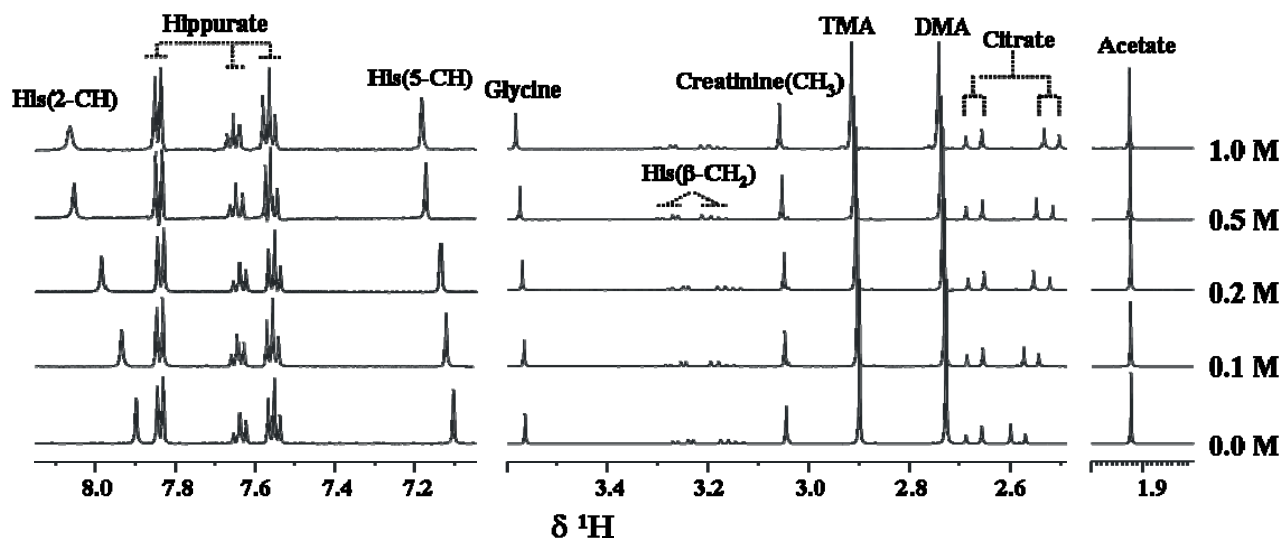


Figure S-2. The ^1H NMR spectra for mixture solutions with different salt concentrations at pH ~ 7.40 .

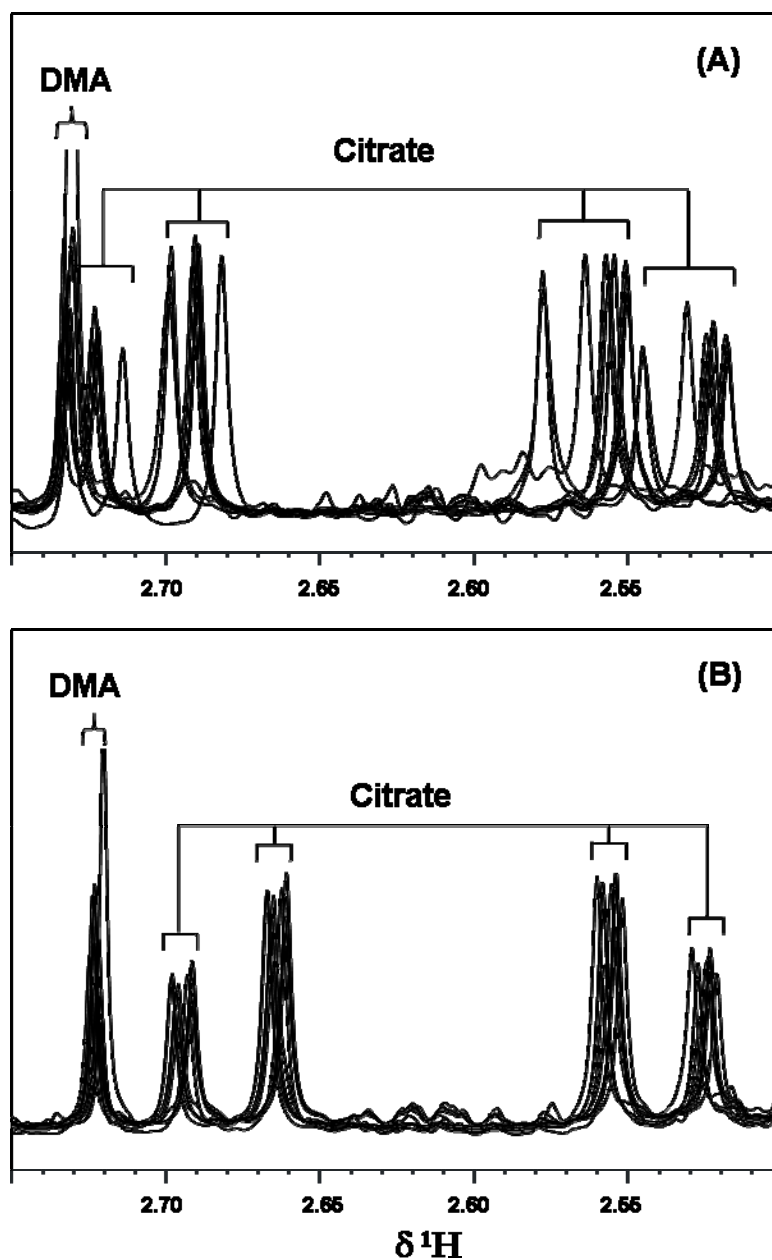


Figure S-3. The chemical shift variations in ^1H NMR spectra (δ 2.75–2.50) for 10 human urine samples, (A) with no added buffer and (B) with the final buffer concentration (C_{FB}) of 0.136 M.